

The 1-D Schrodinger equation is;

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)} \quad (1)$$

This equation determines the solution of a 1-D problem of a particle of mass m moving in potential $V(x)$.

The different constants in the equation are:

\hbar = Planck constant.

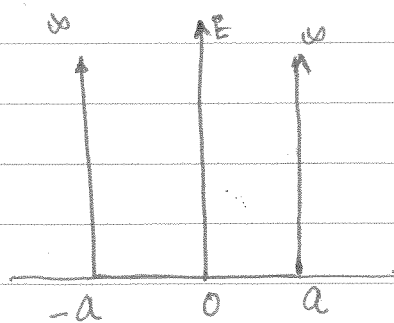
E = Total energy.

ψ = wavefunction describing the system.

= solution $\psi(x)$ which we are looking for.

$\psi^*\psi dx$ = Probability of finding the particle between x and $x+dx$.

For an infinite square well.



$$V(x) = \begin{cases} 0 & , -a \leq x \leq a \\ \infty & ; \text{otherwise} \end{cases}$$

S.E. solved in the interval $-a \leq x \leq a$ gives the solution

$$\psi(x) = A \sin kx + B \cos kx$$

$$\text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

For $-a \leq x \leq a$, $V = \infty$, so the particle should not be found there.

What are the Boundary conditions?

When I said, the particle is not found outside the well, then it means that the wavefunction is zero in that region.

Also, Probability of finding a particle is a continuous function

$\Rightarrow \psi$ must vanish at $x = \pm a$.

Working on with boundary conditions :-

For $x = -a$

$$\psi = -A \sin ka + B \cos ka = 0 \quad \text{--- (2)}$$

For $x = +a$

$$\psi = A \sin ka + B \cos ka = 0 \quad \text{--- (3)}$$

So, adding/subtracting gives us :-

$$B \cos ka = 0 \quad \text{--- (4)}$$

$$A \sin ka = 0 \quad \text{--- (5)}$$

Analysis,

$$A \sin ka = 0$$

$$\text{So, } A = 0 \quad \text{or} \quad \sin ka = 0$$

Let's suppose $A = 0$ is taken

$$\sim B \cos ka = 0, \quad \text{if } B \neq 0 \text{ for soln to exist}$$

$$\Rightarrow \cos ka = 0$$

$$= (2n+1) \frac{\pi}{2}$$

$$n = 0, 1, \dots$$

$$\text{So, } ka = \sqrt{\frac{2mE}{\hbar^2}} a = \left(n + \frac{1}{2}\right) \pi \quad n = 0, 1, \dots$$

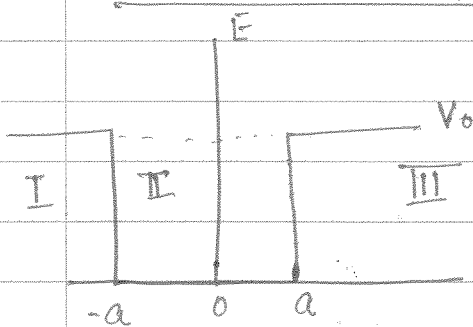
$$\text{or } E_n = \frac{\left(n + \frac{1}{2}\right)^2 \hbar^2 \pi^2}{2ma^2} \quad n = 0, 1, \dots$$

But if $A \neq 0$, then $\sin ka = 0$
 $\Rightarrow ka = 0, \pi, 2\pi, \dots$

$$\Rightarrow E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad n = 1, 2, \dots$$

Infinite = NO

Let's solve for a finite square well potential.



In region I

Schrodinger equation is :-

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (V_0 - E) \psi = 0$$

soln

$$\psi_I(x) = C e^{\beta x} + D e^{-\beta x}$$

$$\beta = \sqrt{\frac{2m}{\hbar^2} (V_0 - E)}$$

Region II

$$\psi_{II} = A \sin \alpha x + B \cos \alpha x$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}}$$

Region III

$$\psi_{III} = F e^{-\beta x}$$

Since $\psi(x)$, $\psi'(x)$ are continuous

At $x = -a$.

$$-A \sin \alpha a + B \cos \alpha a = C e^{-\beta a}$$

and $-\alpha A \cos \alpha a + \alpha B \sin \alpha a = \beta C e^{-\beta a}$

At $x = a$

$$A \sin \alpha a + B \cos \alpha a = F e^{-\beta a}$$

and $\alpha A \cos \alpha a - \alpha B \sin \alpha a = -\beta F e^{-\beta a}$

Let's do this algebra in Matlab

$$\left\{ \begin{array}{l} \text{Even states} \quad A=0, B \neq 0, C=F, \alpha \tan \alpha a = \beta \\ \text{Odd states} \quad A \neq 0, B=0, C=-F, \alpha \cot \alpha a = -\beta \end{array} \right.$$

⚡ Problem of finding energies and ψ of the finite square well has evolved into finding roots of a transcendental equation.